

Benzo[b]thiophene-4-ol

Other names:	Benzo[b]thiophene-4-ol 4-Hydroxybenzothiophene 1-Benzothiophene-4-ol
Inchi:	InChI=1S/C8H6OS/c9-7-2-1-3-8-6(7)4-5-10-8/h1-5,9H
InchiKey:	BMRZGYNNZTVECK-UHFFFAOYSA-N
Formula:	C8H6OS
SMILES:	Oc1cccc2sccc12
Mol. weight [g/mol]:	150.20

Physical Properties

Property code	Value	Unit	Source
hf	-32.48	kJ/mol	Cheméo Relay (1.0)
ie	7.61	eV	Cheméo Relay (1.0)
log10ws	-2.42		Cheméo Relay (1.0)
logp	2.607		Crippen Method
mcvol	106.880	ml/mol	McGowan Method
tb	547.88	K	Cheméo Relay (1.0)
tf	408.49	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3610024&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
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ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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